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A MODEL FOR EXTRINSIC SEMICONDUCTORS WITH DISLOCATIONS IN THE FRAMEWORK OF NON-EQUILIBRIUM THERMODYNAMICS*

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In memory of H. Brezis, an expert in Nonlinear Analysis

Abstract

In this paper, in the framework of rational extended irreversible thermodynamics with internal variables, a model for doped semiconductor crystals with dislocations is worked out, where a dislocation tensor and its gradient are introduced in the set of independent variables to describe these defect lines influencing the mechanical, thermal, electric transport properties of these media. The main equations of the model are introduced and the entropy inequality is analyzed by Liu's theorem, deriving the equations of state for the constitutive variables, the affinities, the dissipation inequality and other relations. Applying Wang's and Smith's theorems the constitutive theory and the expressions for the sources of the rate equations are carried out. According to the extended thermodynamics, a generalized Maxwell-Cattaneo-Vernotte equation for the heat flux and transport equations for the defects and charges fluxes present a relaxation time and a finite velocity for the disturbance propagation. The obtained results may have applications in several technological sectors, such as applied computer science, integrated circuits VLSI and nanotechnology (where high-frequency processes and the construction of sophisticated new materials with particular thermal properties are studied).

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1 Introduction

In some previous papers models for doped semiconductors, also called extrinsic semiconductors, with defects of dislocations (see [23], [49], [50], [29], [30], [31], [32]) were developed in the frame of the rational extended thermodynamics (see [48], [3], [19], [37], [38], [39], [40], [41], [22], [10], [11]) with internal variables [20], [42], [25], [26], [1], [27]. Here, in the same thermodynamic frame a model is carried out for extrinsic semiconductors not electrically polarized and where the dislocation flux tensor is not taken into consideration in the set of independent variables. In particular, in Section 2 doped semiconductors are considered, the influence of the dislocation field, described by a dislocation core tensor *à la Maruszewski* [24] and its gradient, on their thermal and electric behaviour is discussed (see also the models for doped semiconductors with dislocations elaborated in [30], [31], [32]). Maxwell equations, the balance equations of mass, momentum, momentum of momentum and internal energy, and the rate equations for the defects and the heat and charge fluxes are introduced. In Section 3, to describe real non-equilibrium processes, the entropy inequality is analyzed by Liu′s theorem [56] and the laws of state for the constitutive variables, the generalized laws defining the affinities, conjugated to the heat and charges fluxes, the entropy flux and other relations are worked out. Detailed calculations are presented in the Appendix. In Section 4, to close the system of equations describing the behaviour of defective and doped semiconductors under consideration, by virtue Wang's and Smith's theorems (see [60], [61], [62] and [57]) that use isotropic polynomial representations of proper functions obeying the principle of objectivity, the constitutive theory is obtained and the rate equations for the defects field, the charges and heat fluxes, describing physical disturbances with finite velocity, are derived. In particular, a generalized Maxwell-Cattaneo-Vernotte for the heat flux is carried out [2].

The results, obtained in this paper, may have applications in describing the thermal behavior in nanosystems, where the phenomena are fast and the rate of variation of the properties of the system is faster than the time scale characterizing the relaxation of fluxes towards their respective local-equilibrium value. Furthermore, the volume element size d of these nanosystems along some direction is so small that it becomes comparable to

(or smaller than) the mean-free path l of the heat carriers ($d \leq l$).

In defective semiconductors the dislocation lines influence the thermal conductivity and transport coefficients, such as electrical conductivity and Seebeck coefficient.

The models for semiconductor crystals with defects of dislocation (see [49], [50], [52], [12], [13], [14], [15] and [16]) may have relevance in many fundamentals sectors of nanotechnology. One of the main purposes of *defects engineering*, where the influence of dislocations on mechanical and transport properties is investigated, is to obtain a precise control of fluxes in physical systems. The control of the heat flux could be of much current interest in the development of new thermal metamaterials, see [16]. In the review [16] non-equilibrium theories are discussed for heat transport in semiconductors, superlattices, graded systems and metamaterials with defects and some results obtained in this paper were used. In [7], [51], [5], [6] and [52], [12], [53], [54] piezoelectrics and materials with dislocation defects were studied using the same internal variable, its gradient and its flux.

2 The model

In this Section, in the framework of rational extended irreversible thermodynamics with internal variables, we present the equations governing the behaviour of doped semiconductor crystals with dislocations, in a current configuration Kt (see [30], [31], [32] and [54]). For some remarks about the internal variables and some versions of non-equilibrium thermodynamics see for instance Section 2 of Reference [55].

We use the Cartesian tensor notation in a rectangular coordinate system.

The electrical properties of intrinsic semiconductors, as Germanium and Silicon, can be modified using various techniques of "doping". For instance, doping the semiconductors by pentavalent impurities, as antimony, n-type extrinsic semiconductors are obtained, having more flowing free electrons, doping the semiconductors by trivalent impurities, as indium, p-type extrinsic semiconductors are obtained, having more free holes (see [30], [31], [32] and [17], [18]).

In defective semiconductors dislocation channels modify the thermal conductivity. The dislocations density has only a minor effect on the thermal conductivity for defects densities smaller than a characteristic value, but for higher values the thermal conductivity decreases. Therefore, dislocations increase Seebeck thermoelectric coefficient in some range of dislocation densities and for some ranges of dislocation density the efficiency of thermoelec-

tric energy conversion may be raised by dislocations, especially in structures as films, wires.

A relatively high temperature gradient could produce, for instance, a migration of defects inside the system. The dislocation lines disturb the periodicity of the crystal lattice and their structure resembles a network of infinitesimally thin channels (see [9], [47]). Thus, we introduce a dislocation core tensor *à* la Maruszewski (see [24] for its definition, developed in analogy with the structural permeability tensor by Kubik [21]) and its gradient in the thermodynamic state space as internal variables for describing these defects.

Thus, let us consider an elementary sphere volume Ω of a material system with dislocations, large enough to allow the statistical procedures to be applied. Ω is given by $\Omega = \Omega^s + \Omega^c$, where Ω^s is the solid space and Ω^c is the channel space (see [24] and for instance [30], [31], [32]). We assume that the coefficient $f_v = \frac{\Omega^c}{\Omega}$ remains constant inside the medium. Also, we introduce the central section Γ of this elementary sphere volume Ω, being $\Gamma = \Gamma^s + \Gamma^c$, with Γ^s the solid area and Γ^c the dislocation channels area. In such a medium Maruszewski defines the so called dislocation tensor as a linear mapping between the average of a property of some scalar, vector, tensorial physical field $\bar{\alpha}(\mathbf{x})_i$ calculated in the bulk volume Ω and the average $\overset{*}{\alpha}_j(\mathbf{x})$ of the same quantity calculated on the dislocation channels area Γ^c

$$\bar{\alpha}(\mathbf{x})_i = \mathcal{A}_{ij}(\mathbf{x})\, \overset{*}{\alpha}_j(\mathbf{x}) \quad (i, j = 1, 2, 3), \tag{1}$$

where the quantities $\bar{\alpha}(\mathbf{x})_i$ and $\overset{*}{\alpha}_j(\mathbf{x})$ (referred to a Cartesian coordinate system x_i) describe at macroscopic level the property of the physical field under consideration. Furthermore, a new tensor a_{ij}, called *dislocation core tensor*, having unit m^{-2} and referring to the sphere central section Γ is defined as

$$a_{ij}(\mathbf{x}) = \Gamma^{-1}\mathcal{A}_{ij}(\mathbf{x}) \quad (i, j = 1, 2, 3). \tag{2}$$

The dislocation core tensor is a symmetric tensor.

To describe the behaviour of a doped semiconductor crystal with dislocations, let us assume that the following fields interact with each other inside this semiconductor, supposed isotropic and not electrically polarized: the elastic field described by the stress tensor τ_{ij} (in Section 3 we will see that τ_{ij} is symmetric) and the symmetric small-strain tensor ε_{ij}, defined by $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ (where a comma in lower indices denotes the partial spatial derivate, i.e. $u_{i,j} = \frac{\partial u_i}{\partial x_j}$, in vector form $u_{i,j} = [\nabla \mathbf{u}]_{ij}$, being the symbol "$\nabla$" the gradient operator); the thermal field described by the temperature T, its gradient $T_{,i}$ and the heat flux q_i; the electromagnetic field described

by the electric field $\mathcal{E}_i$ and the magnetic induction B_i; the charges fields described by the concentrations (or mass fractions) of electrons n and holes p, their gradients and their currents j_i^n and j_i^p; the dislocation field described by the dislocation core tensor a_{ij} and its gradient $a_{ij,k}$. The independent variables are represented by the set

$$C = \{\varepsilon_{ij}, \mathcal{E}_i, B_i, n, p, T, a_{ij}, j_i^n, j_i^p, q_i, n_{,i}, p_{,i}, T_{,i}, a_{ij,k}\}\,. \tag{3}$$

The physical processes occurring in the above defined situation are governed by three groups of laws: i) the classical balances of mass, momentum, moment of momentum and energy; ii) Maxwell equations; iii) the charges conservation laws, the rate equations of the internal variable a_{ij}, the electric charges fluxes j_i^n, j_i^p and the heat flux q_i. This specific choice shows that the relaxation properties of the thermal field and charge carrier fields are taken into account. However, the corresponding effect for the mechanical properties is not taken into consideration so that τ_{ij} is not in the set (3).

The *continuity equation* reads

$$\dot{\rho} + \rho v_{i,i} = 0, \tag{4}$$

where the superimposed dot indicates the material derivative d/dt, defined by $\frac{d}{dt} = \frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x_i}$, with $\frac{\partial}{\partial t}$ and $\frac{\partial}{\partial x_i}$ the partial temporal derivative and the partial spatial derivative, v_i and ρ are the barycentric velocity and the mass density, respectively, of the whole body, the elastic semiconductor in the considered case. The charge carriers mass has been neglected compared to ρ and in the following we assume that ρ is a constant quantity.

The *momentum balance* has the form

$$\rho\dot{v}_i - \tau_{ji,j} - \rho Z \mathcal{E}_i - \widetilde{\varepsilon}_{ijk}\left(j_j^n + j_j^p\right) B_k, - f_i = 0, \tag{5}$$

where $\widetilde{\varepsilon}_{ijk}$ is the Levi-Civita pseudo-tensor, f_i is the body force, that will be disregarded in the following, $\mathcal{E}_i$ is the electric field E_i referred to the so called comoving frame $\mathcal{K}_c$, given by

$$\mathcal{E}_i = E_i + \widetilde{\varepsilon}_{ijk} v_j B_k$$

and $\mathbf{B}$ is the magnetic induction. Furthermore, in (5) Z is the concentration of the total charge defined as follows:

$$Z = n + \bar{n} + p + \bar{p}, \tag{6}$$

where $n < 0$, $\bar{n} < 0$, $p > 0$, $\bar{p} > 0$.

In (6) n is the concentration of the total negative electric charge given by the concentration of the free electrons coming from doping the semiconductor by pentavalent impurities, denoted by N, and the concentration of the free electrons of the semiconductor intrinsic base, denoted by $\tilde{n}$, namely $n = N + \tilde{n}$; $\bar{n}$ is the charge concentration of fixed negatively ionized atoms of doping trivalent impurities. Furthermore, in (6) p is the concentration of the total positive electric charge given by the concentration of the holes produced by doping the semiconductor by trivalent impurities, denoted by P, and the concentration of the holes coming from the semiconductor intrinsic base, denoted by $\tilde{p}$, namely $p = P + \tilde{p}$; $\bar{p}$ is the charge concentration of fixed positively ionized atoms of doping pentavalent impurities.

The *momentum of momentum balance* is assumed in the form

$$\widetilde{\varepsilon}_{ijk}\tau_{jk} + c_i = 0, \tag{7}$$

where c_i is the couple for unit volume. It will demonstrate in Section 4 that this couple is vanishing, so that the stress tensor τ_{ij} is symmetric.

The *internal energy balance* takes the form

$$\rho\dot{U} - \tau_{ji}v_{i,j} - \left(j_j^n + j_j^p\right)\mathcal{E}_j + q_{i,i} - \rho r = 0, \tag{8}$$

where U is the internal energy density and r is the heat source, that will be neglected in the following.

Maxwell's equations have the form [3], [28]

$$\widetilde{\varepsilon}_{ijk}E_{k,j} + \frac{\partial B_i}{\partial t} = 0, \qquad D_{i,i} - \rho Z = 0, \tag{9}$$

$$\widetilde{\varepsilon}_{ijk}H_{k,j} - j_i^Z - \frac{\partial D_i}{\partial t} = 0, \qquad B_{i,i} = 0, \tag{10}$$

where $\mathbf{D}$, $\mathbf{H}$ and $\mathbf{B}$ are the electric displacement, the magnetic displacement and magnetic field per unit volume, respectively, and $\mathbf{j}^Z$ is the total electric current. Moreover, it has been assumed that the magnetic and dielectric properties of the semiconductor are disregarded, so that the magnetization and the polarization of the material are null, and then $H_i = \frac{1}{\mu_0}B_i$, $E_i = \frac{1}{\varepsilon_0}D_i$, with ε_0 and μ_0 the permittivity and permeability of vacuum, respectively.

To specify the meaning of $\mathbf{j}^Z$ we present an analysis of charge conservation laws (see for instance the models in [23], [30], [31], [32]). In particular, we have

$$\rho\dot{N} + j_{i,i}^N = g^N, \qquad \rho\dot{\tilde{n}} + j_{i,i}^{\tilde{n}} = g^{\tilde{n}}, \quad \rho\dot{\bar{n}} = g^{\bar{n}}, \tag{11}$$

where g^N, $g^{\tilde{n}}$, and $g^{\bar{n}}$ are source terms and it has been taken into consideration that $\bar{n}$ is the charge concentration of fixed negatively ionized atoms with $j_i^{\bar{n}} = 0$.
The concentration $\bar{n}$ is constant, then one has $\dot{\bar{n}} = 0, \quad g^{\bar{n}} = 0$ and from (11) we obtain

$$\rho\dot{n} + j_{i,i}^n = g^n, \tag{12}$$

where $n = N + \tilde{n}$,

$$j_{i,i}^n = j_{i,i}^N + j_{i,i}^{\tilde{n}} \qquad \text{and} \qquad g^n = g^N + g^{\tilde{n}}.$$

Also, we have

$$\rho\dot{P} + j_{i,i}^P = g^P, \qquad \rho\dot{\tilde{p}} + j_{i,i}^{\tilde{p}} = g^{\tilde{p}}, \quad \rho\dot{\bar{p}} = g^{\bar{p}}, \tag{13}$$

where $g^P, g^{\tilde{p}}$, $g^{\bar{p}}$ are source terms and it has been into consideration that $\bar{p}$ is the charge concentration of fixed positively ionized atoms with $j_i^{\bar{p}} = 0$. The concentration $\bar{p}$ is constant. Hence, $\dot{\bar{p}} = 0$, $g^{\bar{p}} = 0$ and from (13) we derive

$$\rho\dot{p} + j_{i,i}^p = g^p, \tag{14}$$

where $p = P + \tilde{p}$,

$$j_{i,i}^p = j_{i,i}^P + j_{i,i}^{\tilde{p}} \qquad \text{and} \qquad g^p = g^P + g^{\tilde{p}}.$$

Moreover, g^n and g^p describe the recombination of electrons and holes and satisfy the equation

$$g^n + g^p = 0.$$

Thus, the total electric current $\mathbf{j}^Z$ is given by

$$j_i^Z = \rho n v_i^n + \rho p v_i^p =$$

$$\rho Z v_i + j_i^n + j_i^p, \tag{15}$$

with

$$\rho Z v_i = \rho(n+p)v_i, \quad j_i^n = \rho n(v_i^n - v_i), \quad j_i^p = \rho p(v_i^p - v_i), \tag{16}$$

(being $v_i^{\bar{n}} = 0$ and $v_i^{\bar{p}} = 0$) where j_i^n, j_i^p are the currents due to the relative motion of ρn and ρp respect to the barycentric motion of the body and Z_i is given by (6). The sum of j_i^n and j_i^p gives the conduction electric current, $\rho Z v_i$ is the convection electric current. The last group of laws concerns the evolution equations of dislocation field, charge fluxes and heat

flux. These rate equations are constructed obeying the objectivity and frame-indifference principles [58], [59], [46], [8], [43] and thus the objective Zaremba-Jaumann derivative is used.

The *rate equation for the dislocation field* is chosen having the form

$$\overset{*}{a}_{ij} + \mathcal{V}_{ijk,k} - A_{ij}(C) = 0, \tag{17}$$

where $A_{ij}(C)$ is the dislocation source (depending on the independent variables) and $\mathcal{V}_{ijk}$ is the dislocation flux tensor, that in the following is supposed having the form $\mathcal{V}_{ijk} = -D' a_{ij,k}$, with D' a dislocation transport coefficient; the *rate equations for the charges* are chosen in the form

$$\overset{*}{j^n}_i = J_i^n(C),$$

$$\overset{*}{j^p}_i = J_i^p(C), \tag{18}$$

where $J_i^n(C)$ and $J_i^p(C)$ are the corresponding charge sources, constitutive functions of the independent variables.

The *rate equation for the heat flux* is assumed having the form

$$\overset{*}{q}_i = Q_i(C), \tag{19}$$

where $Q_i(C)$ is the heat source, constitutive function of the independent variables. In equations (17)-(19), the symbol (*) denotes the Zaremba-Jaumann derivative, respectively, given by

$$\overset{*}{a}_{ij} = \dot{a}_{ij} - w_{ik} a_{kj} - w_{jk} a_{ki},$$

$$\overset{*}{j^n}_i = \dot{j^n}_i - w_{ik} j_k, \quad \overset{*}{j^p}_i = \dot{j^p}_i - w_{ik} j_k, \quad \overset{*}{q}_i = \dot{q}_i - w_{ik} q_k,$$

where $w_{ik} = 1/2(v_{i,k} - v_{k,i})$ is the antisymmeric part of the velocity gradient [43]. In equations (17)-(19) the fluxes of electrons, holes and heat fluxes are not taken into consideration, because we have to obtain a balanced system of equations, where the number of equations is equal to the number of variables.

3 Entropy inequality analysis

To describe real non-equilibrium processes all the admissible solutions of the proposed balance equations and evolution equations should be restricted by the *entropy inequality*, that in the field formulaton has the form

$$\sigma := \rho \dot{S} + \phi_{k,k} - \frac{\rho r}{T} \geq 0, \tag{20}$$

and runs as follows:"the entropy production σ is not negative at each position for all times". In (20) S is the entropy per unit mass, ϕ_k is the entropy flux and $\frac{\rho r}{T}$ is the external source of the entropy production, that will be neglected in the following. A medium is in a state of thermodynamic equilibrium if the entropy production vanishes. Also, equation (20) is a different way to write the second law of thermodynamics, that with its emendment: "Except in equilibrium, there are no reversible process in the state space" states that all local solutions of the balance equations and evolution equations have to satisfy the dissipation inequality (20)(see [38], [39], [44], [45], [35]). If we consider the following set of constitutive functions (dependent variables on the fields of the set C (see (3))

$$W = \{\tau_{ij}, c_i, U, g^n, g^p, A_{ij}, J_i^n, J_i^p, Q_i, S, F, \phi_i, \mu^n, \mu^p, \pi_{ij}\}, \tag{21}$$

with μ^n and μ^p the electrochemical potentials for electrons and holes, respectively, and π_{ij} the potential related to the dislocation field, then we will look for general constitutive equations in the form

$$W = \tilde{W}(C), \tag{22}$$

with both C and W evaluated at the same point and time. The principle of equipresence sates that all constitutive equations depend on the same set of variables of the state space. The axioms of material frame indifference and objectivity also restrict the form of the constitutive functions.

We analyze the entropy inequality (20) by Liu′s procedure [56], where all balance and evolution equations of the problem are considered as mathematical constraints for the general validity of (20). Then, the system of evolution equations (5), (7), (8), (9), (10), (12), (14), (17)-(19) and the entropy inequality (20) can be presented in the form

$$A_{\Delta\gamma} X_\gamma + B_\Delta = 0, \tag{23}$$

$$\alpha_\gamma X_\gamma + \beta \geq 0. \tag{24}$$

Thus, from (23) and (24) applying Liu′s theorem, we have

$$\alpha_\gamma X_\gamma + \beta - \Lambda_\Delta (A_{\Delta\gamma} X_\gamma + B_\Delta) \geq 0, \quad \forall \quad X_\gamma, \tag{25}$$

$$(\alpha_\gamma - \Lambda_\Delta A_{\Delta\gamma}) X_\gamma + (\beta - \Lambda_\Delta B_\Delta) \geq 0, \quad \forall \quad X_\gamma \tag{26}$$

and then

$$\alpha_\gamma - \Lambda_\Delta A_{\Delta\gamma} = 0, \qquad \beta - \Lambda_\Delta B_\Delta \geq 0, \quad \forall \quad X_\gamma, \tag{27}$$

where the so called Lagrange-Liu multipliers Λ_Δ, accounting for the balance equations of momentum and internal energy, Maxwell's equations, the charges conservation equations and the evolution equations of the dislocations field, the charges fluxes and the heat flux (5), (7), (8), (9),(10), (12), (14) and (17)-(19), are objective functions defined by

$$\{\Lambda_\Delta\} = \{\Lambda_i^v, \Lambda^U, \Lambda_i^E, \Lambda_4^E, \Lambda_i^B, \Lambda_4^B, \Lambda^n, \Lambda^p, \Lambda_{ij}^a, \Lambda_i^{j^n}, \Lambda_i^{j^p}, \Lambda_i^q\}. \tag{28}$$

The mass conservation law is not considered, because the density of the semiconductors under consideration is supposed constant. Therefore, if the left-hand side of the laws (5), (7), (8), (9),(10), (12),(14) and (17)-(19) are denoted, respectively, by

$$\mathcal{F}_i^v, \mathcal{F}^U, \mathcal{F}_i^E, \mathcal{F}_4^E, \mathcal{F}_i^B, \mathcal{F}_4^B, \mathcal{F}^n, \mathcal{F}^p, \mathcal{F}_{ij}^a, \mathcal{F}_i^{j^n}, \mathcal{F}_i^{j^p}, \mathcal{F}_i^q,$$

the application of Liu′s theorem (25) gives

$$\rho\frac{\partial S}{\partial t} + \rho v_k S_{,k} + \Phi_{k,k} - \big\{\Lambda_i^v \mathcal{F}_i^v + \Lambda^U \mathcal{F}^U + \Lambda_i^E \mathcal{F}_i^E + \Lambda_4^E \mathcal{F}_4^E + \Lambda_i^B \mathcal{F}_i^B + \Lambda_4^B \mathcal{F}_4^B +$$

$$+ \Lambda^n \mathcal{F}^n + \Lambda^p \mathcal{F}^p + \Lambda_{ij}^a \mathcal{F}_{ij}^a + \Lambda_i^{j^n} \mathcal{F}_i^{j^n} + \Lambda_i^{j^p} \mathcal{F}_i^{j^p} + \Lambda_i^q \mathcal{F}_i^q \Big\} \geq 0, \tag{29}$$

i.e.

$$\rho\frac{\partial S}{\partial t} + \rho v_k S_{,k} + (\phi_k)_{,k} - \Lambda_l^v \left(\rho\frac{\partial v_l}{\partial t} + \rho v_j v_{l,j} - \tau_{jl,j} - \widetilde{\varepsilon}_{ljk}(j_j^n + j_j^p)B_k - \rho Z \mathcal{E}_l\right)$$

$$-\Lambda^U \left(\rho\frac{\partial U}{\partial t} + \rho v_i U_{,i} - \tau_{ji} v_{i,j} + q_{i,i} - (j_i^n + j_i^p)\mathcal{E}_i\right)$$

$$-\Lambda_l^E \left(\frac{1}{\mu_0}\widetilde{\varepsilon}_{lji} B_{i,j} - j_l^n - j_l^p - \rho Z v_l - \varepsilon_0 \frac{\partial \mathcal{E}_l}{\partial t} + \varepsilon_0 \widetilde{\varepsilon}_{lij}\frac{\partial v_i}{\partial t} B_j + \varepsilon_0 \widetilde{\varepsilon}_{lji} v_j \frac{\partial B_i}{\partial t}\right)$$

$$-\Lambda_4^E \Big(\varepsilon_0(\mathcal{E}_{i,i} - \widetilde{\varepsilon}_{jik} v_{i,j} B_k - \widetilde{\varepsilon}_{jki} v_k B_{i,j}) - \rho Z\Big)$$

$$-\Lambda_l^B \left(\widetilde{\varepsilon}_{lji}\mathcal{E}_{i,j} - \widetilde{\varepsilon}_{ljs}\widetilde{\varepsilon}_{sik} v_{i,j} B_k - \widetilde{\varepsilon}_{ljs}\widetilde{\varepsilon}_{ski} v_k B_{i,j} + \frac{\partial B_l}{\partial t}\right)$$

$$-\Lambda_4^B B_{i,i}$$

$$-\Lambda^n\left(\rho\frac{\partial n}{\partial t}+\rho v_i n_{,i}+j^n_{i,j}\delta_{ij}-g^n\right)$$
$$-\Lambda^p\left(\rho\frac{\partial p}{\partial t}+\rho v_i p_{,i}+j^p_{i,j}\delta_{ij}-g^p\right)$$
$$-\Lambda^a_{pl}\left(\frac{\partial a_{pl}}{\partial t}+v_k a_{pl,k}+\frac{\partial \varepsilon_{ps}}{\partial t}a_{sl}-v_{p,s}a_{sl}+\frac{\partial \varepsilon_{sl}}{\partial t}a_{ps}-v_{s,l}a_{ps}-D'a_{pl,kk}-A_{pl}\right)$$
$$-\Lambda^{j^n}_i\left(\frac{\partial j^n_i}{\partial t}+v_j j^n_{i,j}+\frac{\partial \varepsilon_{ij}}{\partial t}j^n_j-v_{i,j}j^n_j-J^n_i\right)$$
$$-\Lambda^{j^p}_i\left(\frac{\partial j^p_i}{\partial t}+v_j j^p_{i,j}+\frac{\partial \varepsilon_{ij}}{\partial t}j^p_j-v_{i,j}j^p_j-J^p_i\right)$$
$$-\Lambda^Q_i\left(\frac{\partial q_i}{\partial t}+v_j q_{i,j}+\frac{\partial \varepsilon_{ij}}{\partial t}q_j-v_{i,j}q_j-Q_i\right)\geq 0, \tag{30}$$

where the mass force and the heat source have been neglected.

Taking into account that the entropy function S, the stress tensor τ_{ij}, the entropy flux ϕ_i, the internal energy U are constitutive functions of the independent variables $\varepsilon_{ij}, \mathcal{E}_i, B_i, n, p, T, a_{ij}, j^n_i, j^p_i, q_i, n_{,i}, p_{,i}, T_{,i}, a_{ij,k}$, performing the calculations from (25) and (30) we derive the following quantities

$$\{\alpha_\gamma\}=\Bigg\{0;\ \rho\frac{\partial S}{\partial \varepsilon_{ij}};\ \rho\frac{\partial S}{\partial \mathcal{E}_i};\ \rho\frac{\partial S}{\partial B_i};\ \rho\frac{\partial S}{\partial n};\ \rho\frac{\partial S}{\partial p};\ \rho\frac{\partial S}{\partial T};\ \rho\frac{\partial S}{\partial a_{ij}};\ \rho\frac{\partial S}{\partial j^n_i};\ \rho\frac{\partial S}{\partial j^p_i};$$
$$\rho\frac{\partial S}{\partial q_i};\ \rho\frac{\partial S}{\partial n_{,i}};\ \rho\frac{\partial S}{\partial p_{,i}};\ \rho\frac{\partial S}{\partial T_{,i}};\ \rho\frac{\partial S}{\partial a_{ij,k}};\ 0;\ \rho v_k\frac{\partial S}{\partial \varepsilon_{ij}}+\frac{\partial \phi_k}{\partial \varepsilon_{ij}};$$
$$\rho v_k\frac{\partial S}{\partial \mathcal{E}_i}+\frac{\partial \phi_k}{\partial \mathcal{E}_i};\ \rho v_k\frac{\partial S}{\partial B_i}+\frac{\partial \phi_k}{\partial B_i};\ \rho v_k\frac{\partial S}{\partial j^n_i}+\frac{\partial \phi_k}{\partial j^n_i};$$
$$\rho v_k\frac{\partial S}{\partial j^p_i}+\frac{\partial \phi_k}{\partial j^p_i};\ \rho v_k\frac{\partial S}{\partial q_i}+\frac{\partial \phi_k}{\partial q_i};\ \rho v_k\frac{\partial S}{\partial n_{,i}}+\frac{\partial \phi_k}{\partial n_{,i}};$$
$$\rho v_k\frac{\partial S}{\partial p_{,i}}+\frac{\partial \phi_k}{\partial p_{,i}};\ \rho v_k\frac{\partial S}{\partial T_{,i}}+\frac{\partial \phi_k}{\partial T_{,i}};\ \rho v_r\frac{\partial S}{\partial a_{ij,k}}+\frac{\partial \phi_r}{\partial a_{ij,k}}\Bigg\}; \tag{31}$$

$$\{X_\gamma\}=\Bigg\{\frac{\partial v_i}{\partial t};\ \frac{\partial \varepsilon_{ij}}{\partial t};\ \frac{\partial \mathcal{E}_i}{\partial t};\ \frac{\partial B_i}{\partial t};\ \frac{\partial n}{\partial t};\ \frac{\partial p}{\partial t};\ \frac{\partial T}{\partial t};\ \frac{\partial a_{ij}}{\partial t};\ \frac{\partial j^n_i}{\partial t};\ \frac{\partial J^p_i}{\partial t};\ \frac{\partial q_i}{\partial t};\frac{\partial n_i}{\partial t};$$
$$\frac{\partial p_i}{\partial t};\ \frac{\partial T_{,i}}{\partial t};\ \frac{\partial a_{ij,k}}{\partial t};\ v_{i,j};\ \varepsilon_{ij,k};\ \mathcal{E}_{i,j};\ B_{i,j};\ j^n_{i,j};\ j^p_{i,j};\ q_{i,j};\ n_{,ij};\ p_{,ij};\ T_{,ij};\ a_{ij,kl}\Bigg\}^T; \tag{32}$$

$$\beta = \left(\rho v_k \frac{\partial S}{\partial n} + \frac{\partial \phi_k}{\partial n}\right) n_{,k} + \left(\rho v_k \frac{\partial S}{\partial p} + \frac{\partial \phi_k}{\partial p}\right) p_{,k} +$$

$$\left(\rho v_k \frac{\partial S}{\partial T} + \frac{\partial \phi_k}{\partial T}\right) T_{,k} + \left(\rho v_k \frac{\partial S}{\partial a_{ij}} + \frac{\partial \phi_k}{\partial a_{ij}}\right) a_{ij,k}; \tag{33}$$

$$\{B_\Delta\} = \left\{ -\frac{\partial \tau_{kl}}{\partial n} n_{,k} - \frac{\partial \tau_{kl}}{\partial p} p_{,k} - \frac{\partial \tau_{kl}}{\partial T} T_{,k} - \frac{\partial \tau_{kl}}{\partial a_{ij}} a_{ij,k} - \rho Z \mathcal{E}_l - \widetilde{\varepsilon}_{ljk} (j_j^n + j_j^p) B_k; \right.$$

$$\rho v_k \frac{\partial U}{\partial n} n_{,k} + \rho v_k \frac{\partial U}{\partial p} p_{,k} + \rho v_k \frac{\partial U}{\partial T} T_{,k} + \rho v_k \frac{\partial U}{\partial a_{ij}} a_{ij,k} - (j_i^n + j_i^p) \mathcal{E}_i;$$

$$\left. -j_l^n - j_l^p - \rho Z v_l;\ -\rho Z;\ 0;\ 0;\ v_s a_{pl,s} - A_{pl};\ \rho v_i n_{,i} - g^n; \rho v_i p_{,i} - g^p; -J_i^n; -J_i^p; -Q_i \right\}, \tag{34}$$

and a suitable matrix $\{A_{\Delta\gamma}\} = \{A^{m|n}\}$ $(m = 1, ..., 12;\ n = 1, ..., 26)$, whose elements are reported in Appendix.

Thus, according to the first requirement of Liu′s theorem (27), the following results are deduced:

$$\Lambda_r^v \rho \delta_{ir} - \Lambda_r^E \widetilde{\varepsilon}_{rij} B_j = 0,$$

$$\rho \frac{\partial S}{\partial \varepsilon_{ij}} - \Lambda^U \rho \frac{\partial U}{\partial \varepsilon_{ij}} = -\Lambda^U \tau_{ji} - \Lambda_p^B \widetilde{\varepsilon}_{pjs} \widetilde{\varepsilon}_{sil} B_l - \Lambda_4^E \varepsilon_0 \widetilde{\varepsilon}_{jik} B_k$$

$$\rho \frac{\partial S}{\partial \mathcal{E}_i} - \Lambda^U \rho \frac{\partial U}{\partial \mathcal{E}_i} = 0,$$

$$\rho \frac{\partial S}{\partial B_i} - \Lambda^U \rho \frac{\partial U}{\partial B_i} = \Lambda_p^B \delta_{ip} + \Lambda_l^E \varepsilon_0 \widetilde{\varepsilon}_{lji} v_j,$$

$$\rho \frac{\partial S}{\partial n} - \Lambda^U \rho \frac{\partial U}{\partial n} = \rho \Lambda^n,$$

$$\rho \frac{\partial S}{\partial p} - \Lambda^U \rho \frac{\partial U}{\partial p} = \rho \Lambda^p,$$

$$\rho \frac{\partial S}{\partial T} - \Lambda^U \rho \frac{\partial U}{\partial T} = 0,$$

$$\rho \frac{\partial S}{\partial a_{ij}} - \Lambda^U \rho \frac{\partial U}{\partial a_{ij}} = \Lambda_{ij}^a,$$

$$\rho \frac{\partial S}{\partial j_i^n} - \Lambda^U \rho \frac{\partial U}{\partial j_i^n} = \Lambda_i^{j^n},$$

$$\rho \frac{\partial S}{\partial j_i^p} - \Lambda^U \rho \frac{\partial U}{\partial j_i^p} = \Lambda_i^{j^p},$$
$$\rho \frac{\partial S}{\partial q_i} - \Lambda^U \rho \frac{\partial U}{\partial q_i} = \Lambda_i^q,$$
$$\rho \frac{\partial S}{\partial n_{,i}} - \Lambda^U \rho \frac{\partial U}{\partial n_{,i}} = 0,$$
$$\rho \frac{\partial S}{\partial p_{,i}} - \Lambda^U \rho \frac{\partial U}{\partial p_{,i}} = 0,$$
$$\rho \frac{\partial S}{\partial T_{,i}} - \Lambda^U \rho \frac{\partial U}{\partial T_{,i}} = 0,$$
$$\rho \frac{\partial S}{\partial a_{ij,k}} - \Lambda^U \rho \frac{\partial U}{\partial a_{ij,k}} = 0, \tag{35}$$

and still we get

$$\rho v_k \frac{\partial S}{\partial \varepsilon_{ij}} + \frac{\partial \phi_k}{\partial \varepsilon_{ij}} - \Lambda^U \rho v_k \frac{\partial U}{\partial \varepsilon_{ij}} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial \varepsilon_{ij}}$$
$$\rho v_k \frac{\partial S}{\partial \mathcal{E}_i} + \frac{\partial \phi_k}{\partial \mathcal{E}_i} - \Lambda^U \rho v_k \frac{\partial U}{\partial \mathcal{E}_i} = - \Lambda_l^v \frac{\partial \tau_{kl}}{\partial \mathcal{E}_i} + \varepsilon_0 \delta_{ik} \Lambda_4^E + \widetilde{\varepsilon}_{pki} \Lambda_p^B,$$

$$\rho v_k \frac{\partial S}{\partial B_i} + \frac{\partial \phi_k}{\partial B_i} - \Lambda^U \rho v_k \frac{\partial U}{\partial B_i} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial B_i} + \Lambda_p^E \frac{1}{\mu_0} \widetilde{\varepsilon}_{pji} - \Lambda_4^E \varepsilon_0 \widetilde{\varepsilon}_{kli} v_l - \Lambda_p^B \widetilde{\varepsilon}_{pks} \widetilde{\varepsilon}_{sli} v_l + \delta_{ik} \Lambda_4^B, \tag{36}$$

and the other results

$$\rho v_k \frac{\partial S}{\partial j_i^n} + \frac{\partial \phi_k}{\partial j_i^n} - \Lambda^U \rho v_k \frac{\partial U}{\partial j_i^n} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial j_i^n} + \Lambda^n \delta_{ik} + v_k \Lambda_i^{j^n},$$
$$\rho v_k \frac{\partial S}{\partial j_i^p} + \frac{\partial \phi_k}{\partial j_i^p} - \Lambda^U \rho v_k \frac{\partial U}{\partial j_i^p} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial j_i^p} + \Lambda^p \delta_{ik} + v_k \Lambda_i^{j^p},$$

$$\begin{aligned}
&\rho v_k \frac{\partial S}{\partial q_i} + \frac{\partial \phi_k}{\partial q_i} - \Lambda^U \rho v_k \frac{\partial U}{\partial q_i} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial q_i} + \Lambda^U \delta_{ik} + v_k \Lambda_i^q,\\
&\rho v_k \frac{\partial S}{\partial n_{,i}} + \frac{\partial \phi_k}{\partial n_{,i}} - \Lambda^U \rho v_k \frac{\partial U}{\partial n_{,i}} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial n_{,i}},\\
&\rho v_k \frac{\partial S}{\partial p_{,i}} + \frac{\partial \phi_k}{\partial p_{,i}} - \Lambda^U \rho v_k \frac{\partial U}{\partial p_{,i}} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial p_{,i}},\\
&\rho v_k \frac{\partial S}{\partial T_{,i}} + \frac{\partial \phi_k}{\partial T_{,i}} - \Lambda^U \rho v_k \frac{\partial U}{\partial T_{,i}} = -\Lambda_l^v \frac{\partial \tau_{kl}}{\partial T_{,i}},\\
&\rho v_r \frac{\partial S}{\partial a_{ij,k}} + \frac{\partial \phi_r}{\partial a_{ij,k}} - \Lambda^U \rho v_r \frac{\partial U}{\partial a_{ij,k}} = -\Lambda_l^v \frac{\partial \tau_{rl}}{\partial a_{ij,k}} - \Lambda_{pl}^a D' \delta_{pi} \delta_{lj} \delta_{kr}.
\end{aligned} \tag{37}$$

Following [36], from $(35)_7$ one derives for the Lagrange multiplier Λ^U the same result as the one obtained in [36]

$$\Lambda^U = \frac{1}{T(\theta)}, \tag{38}$$

where θ denotes the empirical temperature. From $(36)_3$, the Lagrange multipliers Λ_4^E, Λ_p^B, being independent on the velocity v_k, must be null and also from $(36)_2$ and $(35)_1$ the Lagrange multipliers Λ_r^v, Λ_p^E and Λ_4^B, indipendent on the velocity, are null

$$\Lambda_r^v, \quad \Lambda_4^E = 0, \quad \Lambda_p^B, \quad \Lambda_p^E, \quad \Lambda_4^B = 0. \tag{39}$$

From the second requirement of Liu′s theorem $(27)_2$, the following *residual inequality* is obtained

$$\frac{\partial \phi_k}{\partial a_{ij}} a_{ij,k} + \Lambda^U \mathcal{E}_k (j_k^n + j_k^p) + \Lambda_{ik}^a A_{ik} + \Lambda^n g^n + \Lambda^p g^p + \Lambda_i^{j^n} J_i^n + \Lambda_i^{j^p} J_i^p + \Lambda_i^q Q_i \geq 0, \tag{40}$$

where we have taken into consideration that terms containing the velocity v_k must be null and the fluxes do not depend on scalar variables.

Introducing the free energy F and the flux vector K, defined by

$$F = U - TS \quad \text{and} \quad K_i = \rho F v_i - T\phi_i, \tag{41}$$

into (35)-(37) and using (38)-(39) we obtain the following results
the laws of state

$$\rho \frac{\partial F}{\partial \varepsilon_{ij}} = \tau_{ij}, \qquad \rho \frac{\partial F}{\partial \mathcal{E}_i} = 0, \qquad \frac{\partial F}{\partial n_{,i}} = 0, \qquad \frac{\partial F}{\partial p_{,i}} = 0,$$

$$\rho \frac{\partial F}{\partial B_i} = 0, \; \frac{\partial F}{\partial n} = -T\Lambda^n = \mu^n, \; \frac{\partial F}{\partial p} = -T\Lambda^p = \mu^p, \; \rho \frac{\partial F}{\partial a_{ij}} = -T\Lambda_{ij}^a = \pi_{ij},$$
$$\frac{\partial F}{\partial T} = -S, \qquad \frac{\partial F}{\partial T_{,i}} = 0, \qquad \frac{\partial F}{\partial a_{ij,k}} = 0; \tag{42}$$

the affinities (the variables conjugated to the corresponding fluxes)

$$\rho \frac{\partial F}{\partial j_i^n} = -T\Lambda_i^{j^n} = \Pi_i^n, \; \rho \frac{\partial F}{\partial j_i^p} = -T\Lambda_i^{j^p} = \Pi_i^p, \; \rho \frac{\partial F}{\partial q_i} = -T\Lambda_i^q = \Pi_i^Q. \tag{43}$$

Relations (42) and (43) give the physical meaning of *the remaining Lagrange multipliers*, i.e.

$$\Lambda^n = -\frac{1}{T}\mu^n, \qquad \Lambda^p = -\frac{1}{T}\mu^p, \qquad \Lambda^a_{ij} = -\frac{1}{T}\pi_{ij}, \tag{44}$$

$$\Lambda^{j^n}_i = -\frac{1}{T}\Pi^n_i, \quad \Lambda^{j^p}_i = -\frac{1}{T}\Pi^p_i, \qquad \Lambda^q_i = -\frac{1}{T}\Pi^q_i. \tag{45}$$

The group of relations pertaining to the flux-like properties of the considered processes are:

$$\frac{\partial K_k}{\partial \varepsilon_{ij}} = 0, \qquad \frac{\partial K_k}{\partial \mathcal{E}_i} = 0, \qquad \frac{\partial K_k}{\partial B_i} = 0,$$

$$\frac{\partial K_k}{\partial j^n_i} = \mu^n \delta_{ik} + \Pi^n_i v_k, \qquad \frac{\partial K_k}{\partial j^p_i} = \mu^p \delta_{ik} + \Pi^p_i v_k,$$

$$\frac{\partial K_k}{\partial q_i} = -\delta_{ik} + \Pi^q_i v_k, \qquad \frac{\partial K_k}{\partial n_{,i}} = 0, \qquad \frac{\partial K_k}{\partial p_{,i}} = 0,$$

$$\frac{\partial K_k}{\partial T_{,i}} = 0 \qquad \frac{\partial K_r}{\partial a_{ij,k}} = D'\pi_{ij}\delta_{kr} \tag{46}$$

From these results the *residual inequality* (40) simplifies to

$$T\frac{\partial \phi_k}{\partial a_{ij}} a_{ij,k} + (j^n_k + j^p_k)\mathcal{E}_k - \pi_{ij}A_{ij} - \mu^n g^n - \mu^p g^p - \Pi^n_i J^n_i - \Pi^p_i J^p_i - \Pi^q_i Q_i \geq 0. \tag{47}$$

Integrating expression (46) in a proper way, taking into account (41), (42) and (43), we obtain

$$K_k = -q_k + \mu^n j^n_k + \mu^p j^p_k + D'\pi_{ij}a_{ij,k} + \rho v_k F \tag{48}$$

and the form of the entropy flux given by

$$\phi_k = \frac{1}{T}(q_k - \mu^n j^n_k - \mu^p j^p_k - D'\pi_{ij}a_{ij,k}). \tag{49}$$

From (49) it is seen that in the entropy flux there are the contributions due to the heat flux, the charges fluxes and the dislocation gradient tensor. Also, from (42) and (43) it results that the free energy is given by the following function

$$F = F(\varepsilon_{ij}, n, p, T, a_{ij}, j^n_i, j^p_i, q_i). \tag{50}$$

For the invariance of F under time reversal, the expressions of F contains no first order or odd order terms for the fluxes.

From the state law $(42)_1$ the stress tensor τ_{ij} is symmetric, being ϵ_{ij} symmetric, and therefore in the momentum of momentum balance (7) the couple c_i vanishes. The results obtained in this Section are applied in the following to get the unknown constitutive functions, present in the considered model to describe isotropic doped semiconductors with defects of dislocation.

4 Constitutive theory

In this Section, in order to have a closed system of equations having the same number of equations and physical quantities present in them (independent and dependent variables) [40], by the help of Wang's and Smith's theorems (see [60], [61], [62], [57]), that use isotropic polynomial representations of propre functions satisfying the objectivity principle and the material indifference principles, the constitutive theory and the expressions for the external source terms $A_{ij} = A_{ij}(C)$ and $J_k^n = J_k^n(C)$, $J_k^p = J_k^p(C)$, $Q_k = Q_k(C)$ (present in the rate equations for the dislocation field, electrons, holes and heat fluxes, respectively) are derived, in a first approximation. We suppose that the quantities a_{ij}, A_{ij} and π_{ij} responsible for the dislocation field, influencing mechanical and transport processes within the medium, have the form

$$a_{ij} = a\delta_{ij}, \qquad A_{ij} = A\delta_{ij}, \qquad \pi_{ij} = \pi\delta_{ij}. \tag{51}$$

This assumption can be justified by the fact that by splitting a tensor of second order, for example G_{ij}, in its deviatoric part $\tilde{G}_{ij}$ and its scalar part G (spherical part of G_{ij})

$$G_{ij} = \tilde{G}_{ij} + G\delta_{ij}, \tag{52}$$

with $G = \frac{1}{3}G_{kk}$ and $\tilde{G}_{ij} = G_{ij} - \frac{1}{3}G_{kk}\delta_{ij}$, the deviatoric part of G_{ij} is supposed neglegible.

Therefore, taking into account the laws of state (42), the affinities definitions (43), the form of the free energy (50) (time reversal invariant), that τ_{ij} is a symmetric tensor, $\Pi_i^n, \Pi_i^p, \Pi_i^Q, J_i^n, J_i^p, Q_i$ are polar vectors, S, μ^n, μ^p, π, A are scalars, and the affinities are quantities conjugate to fluxes (polar vectors), the following objective representations are obtained for *the constitutive functions* in a first approximation

$$\tau_{ij} = \tau_{ij}(\varepsilon_{ij}, n, p, T, a), \quad S = S(\varepsilon_{ij}, n, p, T, a), \quad \mu^n = \mu^n(\varepsilon_{ij}, n, p, T, a),$$

$$\mu^p = \mu^p(\varepsilon_{ij}, n, p, T, a), \quad \pi = \pi(\varepsilon_{ij}, n, p, T, a), i.e. \tag{53}$$

$$\tau_{ij} = \beta^1_\tau \delta_{ij} + \beta^2_\tau \varepsilon_{ij}, \tag{54}$$

$$S = \beta^1_s n + \beta^2_s p + \beta^3_s T + \beta^4_s a + \beta^5_s \varepsilon_{ii}, \tag{55}$$

$$\mu^n = \beta^1_n n + \beta^2_n p + \beta^3_n T + \beta^4_n a + \beta^5_n \varepsilon_{ii}, \tag{56}$$

$$\mu^p = \beta^1_p n + \beta^2_p p + \beta^3_p T + \beta^4_p a + \beta^5_p \varepsilon_{ii}, \tag{57}$$

$$\pi = \beta^1_\pi n + \beta^2_\pi p + \beta^3_\pi T + \beta^4_\pi a + \beta^5_\pi \varepsilon_{ii}, \tag{58}$$

where the coefficients β^α_τ, $(\alpha = 1, 2)$ $\beta^\beta_n, \beta^\beta_p, \beta^\beta_s, \beta^\beta_\pi$, $(\beta = 1, 2, ..., 5)$ can be functions of the following invariants

$$n, p, T, a, \varepsilon_{kk}, \varepsilon_{ij}\varepsilon_{ij}, \varepsilon_{ij}\varepsilon_{jk}\varepsilon_{ki}; \tag{59}$$

the affinities

$$\Pi^n_i = \Pi^n_i(j^n_i, j^p_i, q_i), \qquad \Pi^p_i = \Pi^p_i(j^n_i, j^p_i, q_i), \qquad \Pi^q_i = \Pi^q_i(j^n_i, j^p_i, q_i), \tag{60}$$

$$\Pi^n_i = \beta^1_N j^n_i + \beta^2_N j^p_i + \beta^3_N q_i, \tag{61}$$

$$\Pi^p_i = \beta^1_P j^n_i + \beta^2_P j^p_i + \beta^3_P q_i, \tag{62}$$

$$\Pi^q_i = \beta^1_Q j^n_i + \beta^2_Q j^p_i + \beta^3_Q q_i, \tag{63}$$

where β^δ_N, β^δ_P, $\beta^\delta_Q(\delta = 1, 2, 3)$ can depend on the invariants:

$$j^p_i j^p_i, j^n_i j^n_i, j^n_i j^p_i, j^p_i q_i, q_i q_i, j^n_i q_i. \tag{64}$$

Furthermore, representing the external source terms $A_{ij} = A_{ij}(C)$ and $J^n_k = J^n_k(C)$, $J^p_k = J^p_k(C)$, $Q_k = Q_k(C)$, we obtain in a first approximation the rate equations (17), (18) and (19) in the following form

$$\overset{*}{a} - D' a_{,kk} = \gamma^1_a n + \gamma^2_a p + \gamma^3_a T + \gamma^4_a a + \gamma^5_a \varepsilon_{kk}, \tag{65}$$

$$\overset{*}{J}{}^{n}_{k} = \gamma_n^1 \mathcal{E}_i + \gamma_n^2 a_{,k} + \gamma_n^3 n_{,k} + \gamma_n^4 p_{,k} + \gamma_n^5 T_{,k} + \gamma_n^6 j_k^n + \gamma_n^7 j_k^p + \gamma_n^8 q_k, \tag{66}$$

$$\overset{*}{J}{}^{p}_{k} = \gamma_p^1 \mathcal{E}_i + \gamma_p^2 a_{,k} + \gamma_p^3 n_{,k} + \gamma_p^4 p_{,k} + \gamma_p^5 T_{,k} + \gamma_p^6 j_k^n + \gamma_p^7 j_k^p + \gamma_p^8 q_k, \tag{67}$$

$$\overset{*}{q}_{k} = \gamma_q^1 \mathcal{E}_i + \gamma_q^2 a_{,k} + \gamma_q^3 n_{,k} + \gamma_q^4 p_{,k} + \gamma_q^5 T_{,k} + \gamma_q^6 j_k^n + \gamma_q^7 j_k^p + \gamma_q^8 q_k, \tag{68}$$

where the coefficients $\gamma_a^\varepsilon(\varepsilon = 1, 2, ..., 5)$ and $\gamma_n^\omega, \gamma_p^\omega, \gamma_q^\omega(\omega = 1, 2, ..., 8)$ can depend on invariants built on the set C (3).

The reader is advised to read the Appendices of Reference [4], where a representation of objective functions was derived in full details for porous media, starting from considerations on Wang's and Smith's theorems [60], [61], [62], [57].

In the physical situations, where we can replace Zaremba-Jaumannn derivative by the material derivative equations, (65)-(68) take the form

$$\tau^a \dot{a} - D' a_{,kk} = -a + \chi_a^1 n + \chi_a^2 p + \chi_a^3 T + \chi_a^4 \varepsilon_{kk}, \tag{69}$$

$$\tau^{J^n} \dot{j}_k^n = -j_k^n - \lambda^n T_{,k} + \chi^n \mathcal{E}_i + \chi_n^1 a_{,k} + \chi_n^2 n_{,k} + \chi_n^3 p_{,k} + \chi_n^4 j_k^p + \chi_n^5 q_k, \tag{70}$$

$$\tau^{J^p} \dot{j}_k^p = -j_k^p - \lambda^p T_{,k} + \chi^p \mathcal{E}_i + \chi_p^1 a_{,k} + \chi_p^2 n_{,k} + \chi_p^3 p_{,k} + \chi_p^4 j_k^n + \chi_p^5 q_k, \tag{71}$$

$$\tau^q \dot{q}_k = -q_k - \lambda T_{,k} - \chi^q \mathcal{E}_i + \chi_q^1 a_{,k} + \chi_q^2 n_{,k} + \chi_q^3 p_{,k} + \chi_q^4 j_k^n + \chi_q^5 j_k^p, \tag{72}$$

where $\gamma_a^4 = -\tau^{a(-1)}$, $\gamma_q^6 = -\tau^{J^n(-1)}, \gamma_q^7 = -\tau^{J^p(-1)}$ and $\gamma_q^8 = -\tau^{q(-1)}$ are the inverse of the relaxation times of the defects and the electrons, holes, heat fluxes, respectively, see (65) − (68). The new coefficients $D', \lambda^n, \lambda^p, \lambda$, $\chi_a^\delta(\ \delta = 1, 2, 3, 4)$, χ_n^ε, χ_p^ε and $\chi_q^\varepsilon(\ \varepsilon = 1, 2, .., 5)$ in (70) − (72) are expressed in terms of the coefficients present in equations (65) − (68) and the minus signs come from physical reasons. D' represents a diffusion coefficient of defects, λ^n, λ^p are Seebeck coefficients, λ is the thermal conductivity, χ^n, χ^p are conductivities, χ^q is Peltier coefficient. The rate equation for the

heat flux (72) generalizes Vernotte-Cattaneo law $\tau^q \dot{q}_k = -q_k - \lambda T_{,k}$, where the finite velocity of the thermal disturbances is taken into consideration, eliminating the paradox of Fourier heat equation $q_k = -\lambda T_{,k}$, that leads to thermal propagation with infinite velocity. Equations (69) and (71) are new, but the equation (70) is the generalized Fick-Ohm's law concerning relaxation features of the electron field.

5 Conclusions

In this paper a model for isotropic doped defective semiconductor crystals was developed in the framework of the rational extended irreversible thermodynamics with internal variables. Here, the considered semiconductors are not electrically polarized and the dislocations flux tensor is not an independent variable, as in other papers of the author. Also, it was assumed that the mass density is constant, the body force, the heat and the external entropy sources are negligible. The entropy inequality was analyzed by Liu's theorem, where all balance and evolution equations of the problem are considered as mathematical constraints for its validity. The state laws, the affinities, the residual dissipation, the entropy flux and other relations were derived and the results obtained here were used in [13], [14], [15], [16]. In these papers the behaviour of superlattices of doped defective semiconductors was investigated, taking into account the role of the interfaces between their alternative layers, and this behaviour can be used as a basis for the construction of thermal transistors, thermal computers an other devices. Furthermore, in this paper, using Wang's and Smith's theorems objective, constitutive relations and transport equations were constructed in a first approximation. Rate equations, presenting a relaxation time, that describe disturbances having a finite velocity of propagation were derived. It was shown that a field of dislocation lines in an extrinsic semiconductor crystal has influence on its mechanical and heat and electric transport properties. In [33] and [34] weak discontinuity waves and asymptotic electronic-dislocation waves in n-type semiconductors with defects of dislocation were studied by the author using a model similar to the one developed here. The theory elaborated in this paper has several applications in nanotechnology and other technological sectors.

Appendix

In this Appendix we present the elements of the matrix $\{A_{\Delta\gamma}\} = \{A^{m|n}\}$ $(m = 1, ..., 12;\ n = 1, ..., 26)$:

$$A^{1|1} = \rho\delta_{il},\ A^{1|2} = ... = A^{1|15} = 0,\ A^{1|16} = \rho v_j \delta_{il},\ A^{1|17} = -\frac{\partial \tau_{kl}}{\partial \varepsilon_{ij}},$$

$$A^{1|18} = -\frac{\partial \tau_{jl}}{\partial \mathcal{E}_i},\ A^{1|19} = -\frac{\partial \tau_{jl}}{\partial B_i},\ A^{1|20} = -\frac{\partial \tau_{jl}}{\partial j_i^n},\ A^{1|21} = -\frac{\partial \tau_{jl}}{\partial j_i^p},$$

$$A^{1|22} = -\frac{\partial \tau_{jl}}{\partial q_i},\ A^{1|23} = -\frac{\partial \tau_{jl}}{\partial n_{,i}},\ A^{1|24} = -\frac{\partial \tau_{jl}}{\partial p_{,i}},$$

$$A^{1|25} = -\frac{\partial \tau_{jl}}{\partial T_{,i}},\ A^{1|26} = -\frac{\partial \tau_{rl}}{\partial a_{ij,k}},$$

$$A^{2|1} = 0, \quad A^{2|2} = \rho\frac{\partial U}{\partial \varepsilon_{ij}}, \quad A^{2|3} = \rho\frac{\partial U}{\partial \mathcal{E}_i},\ A^{2|4} = \rho\frac{\partial U}{\partial B_i},$$

$$A^{2|5} = \rho\frac{\partial U}{\partial n},\ A^{2|6} = \rho\frac{\partial U}{\partial p},\ A^{2|7} = \rho\frac{\partial U}{\partial T},\ A^{2|8} = \rho\frac{\partial U}{\partial a_{ij}},$$

$$A^{2|9} = \rho\frac{\partial U}{\partial j_i^n},\ A^{2|10} = \rho\frac{\partial U}{\partial j_i^p}, \quad A^{2|11} = \rho\frac{\partial U}{\partial q_i}, \quad A^{2|12} = \rho\frac{\partial U}{\partial n_{,i}},$$

$$A^{2|13} = \rho\frac{\partial U}{\partial p_{,i}}, \quad A^{2|14} = \rho\frac{\partial U}{\partial T_{,i}},\ A^{2|15} = \rho\frac{\partial U}{\partial a_{ij,k}},$$

$$A^{2|16} = -\tau_{ji},\ A^{2|17} = \rho v_k \frac{\partial U}{\partial \varepsilon_{ij}},$$

$$A^{2|18} = \rho v_j \frac{\partial U}{\partial \mathcal{E}_i},\ A^{2|19} = \rho v_j \frac{\partial U}{\partial B_i},\ A^{2|20} = \rho v_j \frac{\partial U}{\partial j_i^n},\ A^{2|21} = \rho v_j \frac{\partial U}{\partial j_i^p},$$

$$A^{2|22} = \rho v_j \frac{\partial U}{\partial q_i} + \delta_{ij},\ A^{2|23} = \rho v_j \frac{\partial U}{\partial n_{,i}},\ A^{2|24} = \rho v_j \frac{\partial U}{\partial p_{,i}},$$

$$A^{2|25} = \rho v_j \frac{\partial U}{\partial T_{,i}},\ A^{2|26} = \rho v_r \frac{\partial U}{\partial a_{ij,k}},$$

$$A^{3|1} = \varepsilon_0 \widetilde{\varepsilon}_{lij} B_j,\ A^{3|2} = 0,\ A^{3|3} = -\varepsilon_0 \delta_{li},\ A^{3|4} = \varepsilon_0 \widetilde{\varepsilon}_{lji} v_j,$$

$$A^{3|5} = ... = A^{3|18} = 0,\ A^{3|19} = \frac{1}{\mu_0}\widetilde{\varepsilon}_{lji},\ A^{3|20} = ... = A^{3|26} = 0,$$

$$A^{4|1} = ... = A^{4|15} = 0,\ A^{4|16} = -\varepsilon_0 \widetilde{\varepsilon}_{jik} B_k,$$

$$A^{4|17} = 0,\ A^{4|18} = \varepsilon_0 \delta_{ij},\ A^{4|19} = -\varepsilon_0 \widetilde{\varepsilon}_{jki} v_k,\ A^{4|20} = 0,$$

$$A^{4|21} = ... = A^{4|26} = 0,$$
$$A^{5|1} = ... = A^{5|3} = 0,\ A^{5|4} = \delta_{il},\ A^{5|5} = ... = A^{5|15} = 0,\ A^{5|16} = -\widetilde{\varepsilon}_{ljs}\widetilde{\varepsilon}_{sik}B_k,$$
$$A^{5|17} = 0,\ A^{5|18} = -\widetilde{\varepsilon}_{lji},\ A^{5|19} = -\widetilde{\varepsilon}_{ljs}\widetilde{\varepsilon}_{ski}v_k,\ A^{5|20} = ... = A^{5|26} = 0,$$
$$A^{6|1} = ... = A^{6|18} = 0,\ A^{6|19} = \delta_{ij},\ A^{6|20} = ... = A^{6|26} = 0,$$
$$A^{7|1} = ... = A^{7|4} = 0,\ A^{7|5} = \rho,\ A^{7|6} = ... = A^{7|19} = 0,$$
$$A^{7|20} = \delta_{ij},\ A^{7|21} = ... = A^{7|26} = 0,$$
$$A^{8|1} = ... = A^{8|5} = 0,\ A^{8|6} = \rho,\ A^{8|7} = ... = A^{8|20} = 0,$$
$$A^{8|21} = \delta_{ij},\ A^{8|22} = ... = A^{8|26} = 0,$$
$$A^{9|1} = 0,\ A^{9|2} = a_{sl}\delta_{pi}\delta_{sj} + a_{ps}\delta_{si}\delta_{lj},\ A^{9|3} ... = A^{9|7} = 0,\ A^{9|8} = \delta_{ip}\delta_{lj},$$
$$A^{9|9} = ... = A^{9|15} = 0,\ A^{9|16} = -a_{sl}\delta_{pi}\delta_{sj} - a_{ps}\delta_{si}\delta_{lj},\ A^{9|17} = ... = A^{9|25} = 0,$$
$$A^{9|26} = -D'\delta_{pi}\delta_{lj}\delta_{kr},$$
$$A^{10|1} = 0,\ A^{10|2} = j^n_j,\ A^{10|3} = ... = A^{10|8} = 0,$$
$$A^{10|9} = 1,\ A^{10|10} = ... = A^{10|15} = 0,$$
$$A^{10|16} = -j^n_j,\ A^{10|17} = ... = A^{11|19} = 0,\ A^{10|20} = v_j,$$
$$A^{10|21} = ... = A^{10|26} = 0,$$
$$A^{11|1} = 0,\ A^{11|2} = j^p_j,\ A^{11|3} = ... = A^{11|9} = 0,\ A^{11|10} = 1;$$
$$A^{11|11} = ... = A^{11|15} = 0,$$
$$A^{11|16} = -j^p_j,\ A^{11|17} = ... = A^{11|20} = 0,\ A^{11|21} = v_j,$$
$$A^{11|22} = ... = A^{11|26} = 0,$$
$$A^{12|1} = 0,\ A^{12|2} = q_j,\ A^{12|3} = ... = A^{12|10} = 0,\ A^{12|11} = 1,$$
$$A^{12|12} = ... = A^{12|15} = 0,$$
$$A^{12|16} = -q_j,\ A^{12|17} = ... = A^{12|21} = 0,\ A^{12|22} = v_j,$$
$$A^{12|23} = ... = A^{12|26} = 0.$$

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